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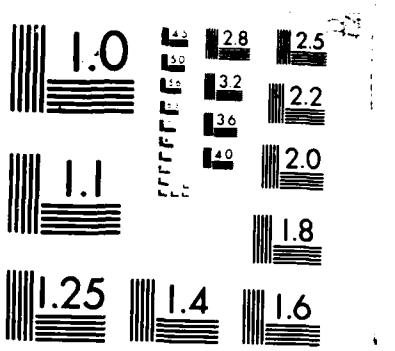

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Rapid Evaluation of Potential Fields in Three Dimensions

L. Greengard and V. Rokhlin

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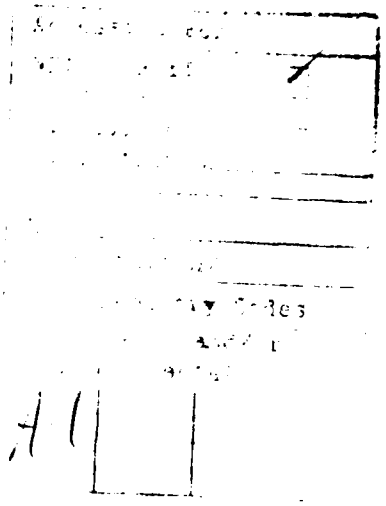
DEPARTMENT OF COMPUTER SCIENCE

This paper describes a three-dimensional version of the fast multipole algorithm ([7],[13],[4]) for the rapid evaluation of the potential and force fields in systems of particles whose interactions are Coulombic or gravitational in nature. For a system of N particles, an amount of work of the order $O(N^2)$ has traditionally been required to evaluate all pairwise interactions, unless some approximation or truncation method is used. The algorithm presented here requires an amount of work proportional to N to evaluate all interactions to within roundoff error, making it considerably more practical for large-scale problems encountered in plasma physics, fluid dynamics, molecular dynamics and celestial mechanics.



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1. Introduction

The evaluation of Coulombic and gravitational interactions in large-scale ensembles of particles is an integral part of the numerical simulation of a large number of physical processes. Typical examples include celestial mechanics, plasma simulations, the vortex method in fluid dynamics, and the solution of the Laplace equation via potential theory (see [10], [5], [14], [2]). In such cases, the potential has the form

$$\Phi = \Phi_{external} + \Phi_{local} + \Phi_{far}, \tag{1.1}$$

where Φ_{local} is a rapidly decaying function of distance (such as the Van der Waals potential in chemical physics), $\Phi_{external}$ is a function which is independent of the number and relative positions of the particles (such as an external gravitational field), and Φ_{far} is Coulombic or gravitational.

In the numerical evaluation of fields of the form (1.1), the cost of computing the terms $\Phi_{external}$ and Φ_{local} is of the order $O(N)$, where N is the number of particles in the ensemble. Indeed, $\Phi_{external}$ is evaluated separately for each particle, and Φ_{local} decays rapidly, involving the interactions of each particle with a small number of nearest neighbors. Unfortunately, evaluation of the term Φ_{far}, if done directly, requires order $O(N^2)$ operations, since the Coulombic potential decays slowly, and the interactions between each pair of particles have to be taken into account. In many situations, in order to be of physical interest, the simulation has to involve thousands of particles (or more), making the estimate $O(N^2)$ excessive in some cases, and prohibitive in others.

Many three-dimensional processes are more or less adequately described by two-dimensional models, and this fact is widely used in computer simulations. From the computational point of view, reduction of the dimensionality of the problem has several major advantages: fewer particles are normally required to obtain a physically meaningful model of a two-dimensional process than that of its three-dimensional counterpart, the numerical techniques for calculations in two dimensions are better developed and easier to implement, and finally, the display and interpretation of three-dimensional results pose problems almost non-existent in two dimensions. On the other hand, certain processes in the physical world simply can not be approximated by two-dimensional models. In such cases, full three-dimensional simulations have to be performed, with the help of appropriate numerical tools.

We restrict our attention now to the evaluation of Coulombic or gravitational potentials, and begin by observing that multipole expansions have been a popular tool in the analysis of such problems for more than 100 years ([11],[12]). They are routinely used to represent the fields due to collections of charges (masses) in regions of space removed from the source positions. However, these classical techniques are generally inapplicable in situations where the charges and the points where the fields are to be evaluated are not separated. The use of multipole expansions for the evaluation of fields in such a situation was reported in [14], where the solution of the Laplace equation by means of boundary integrals is discussed. The method described requires the evaluation of the potential field induced by a collection of N charges lying on a curve at each of the charge locations, and a multipole-based algorithm is used to carry out this calculation in order $O(N)$ operations. In [7],[8], we introduced a generalization of this method for the rapid evaluation of the potentials and forces in large-scale two-dimensional systems of particles randomly distributed in a square domain. This fast multipole algorithm requires an amount of work proportional to N to evaluate to within round-off error all pairwise interactions in a system of N charges. In [4], an adaptive version of the algorithm of [7],[8] was introduced, whose CPU time requirements are proportional to N and independent of the statistics of the charge distribution.

This paper reports the theoretical apparatus underlying the three-dimensional version of the fast multipole algorithm. For a full description of the method in three dimensions, as well as a

detailed discussion of numerical results produced by implementations of the method in two dimensions, we refer the reader to [13]. Other aspects of the problem discussed in [13] include applications of the method to several problems in physics, chemistry, and biology.

While in [7],[8] the analytical foundation is the theory of holomorphic functions, here it is the theory of spherical harmonics. Conceptually, the transition is quite straightforward. However, a number of technical problems had to be overcome before an efficient three-dimensional algorithm could be constructed. In particular, we formulate and prove two generalizations of the classical addition theorem for the Legendre polynomials (Theorems 2.3 and 2.4 of this paper) that appear to have been previously unknown.

Remark: Several other approaches have been used to reduce the cost of the evaluation of Coulombic potential fields. For a detailed discussion of these algorithms, we refer the reader to [7], and to the original works [10], [1], [2].

2. Physical and Mathematical Preliminaries

In this paper, we will be considering three-dimensional physical models, consisting of a set of N charged particles with the potential and force obtained as the sum of pairwise interactions via Coulomb's law. If a point charge of unit strength is located at the origin, then for any point $P = (x, y, z) \in \mathbf{R}^3$ with $\|P\| = r \neq 0$, the potential and electrostatic field due to this charge are described by the expressions

$$\Phi = \frac{1}{r} \qquad \text{and}$$
$$\vec{E} = -\nabla\Phi = \left(\frac{x}{r^3}, \frac{y}{r^3}, \frac{z}{r^3}\right) ,$$

respectively.

Using spherical coordinates, suppose now that the unit charge is located at a point $Q = (\rho, \alpha, \beta)$, not the origin. The potential at a point $P \neq Q$ is, of course, the inverse of the distance $\|P - Q\| = r'$ (Figure 1). There is a well-known series expansion for the potential at $P = (r, \theta, \phi)$, in terms of its distance from the origin r. Letting γ be the angle between the vectors P and Q, we have

$$\frac{1}{r'} = \sum_{n=0}^{\infty} \frac{\rho^n}{r^{n+1}} P_n(u) , \tag{2.1}$$

where $u = \cos\gamma$ and $P_n(u)$ is the Legendre polynomial of degree n. Equation (2.1) is generally referred to as a multipole expansion, and describes the far field due to a charge at Q, since the condition for its validity is that $r > \rho$.

There is a duality inherent in the situation depicted in Figure 1, namely that if the locations of the charge (Q) and the evaluation point (P) were interchanged, then the field at P would still be described by $\frac{1}{r'}$. In this case, so long as $r < \rho$, we may write

$$\frac{1}{r'} = \sum_{n=0}^{\infty} \frac{r^n}{\rho^{n+1}} P_n(u). \tag{2.2}$$

Equation (2.2) is valid only in the open sphere centered at the origin with radius ρ, and we will refer to such a description of the potential field as a local expansion.

The following observation pertaining to Legendre polynomials will be needed below. Its proof can be found in most standard textbooks (see, for example, [11]).

Lemma 2.1. *Let $u \in \mathbf{R}$, with $|u| \leq 1$. Then $P_n(u) \leq 1$.*

From this fact, it is straightforward to obtain the following two error bounds.

Lemma 2.2. *Suppose that a charge of strength q is located at the point $Q = (\rho, \alpha, \beta)$, and that $P = (r, \theta, \phi) \in \mathbf{R}^3$, with $\|P - Q\| = r'$ and $r > \rho$. Letting γ be the angle between the two points, we have an error bound for the multipole expansion (2.1) of the form*

$$\left| \frac{q}{r'} - \sum_{n=0}^{p} \frac{q \cdot \rho^n}{r^{n+1}} P_n(\cos\gamma) \right| \leq \frac{q}{r - \rho} \left(\frac{\rho}{r} \right)^{p+1} . \tag{2.3}$$

Similarly, when $r < \rho$, we have an error bound for the local expansion (2.2) of the form

$$\left| \frac{q}{r'} - \sum_{n=0}^{p} \frac{q \cdot r^n}{\rho^{n+1}} P_n(\cos\gamma) \right| \leq \frac{q}{\rho - r} \left(\frac{r}{\rho} \right)^{p+1} . \tag{2.4}$$

Examining equation (2.1) yet again, we note that the resulting series depends on the relative coordinates of the two particles. If another such series were developed for a second source at the point Q', they would have to be evaluated independently. We will therefore need a more general approach to the solution of potential problems, which will allow us to develop asymptotic expansions of the field due to arbitrary sets of charges.

2.1. Spherical Harmonics

The development of a general expansion describing potential fields in three dimensions is carried out by considering the Laplace equation itself, which characterizes the behavior of such fields in regions of free space. Using spherical coordinates, the Laplace equation takes the form

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0.$$

The standard solution of this equation by separation of variables results in an expression for the field as a series, the terms of which are known as spherical harmonics.

$$\Phi(r, \theta, \phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(L_n^m \cdot r^n + \frac{M_n^m}{r^{n+1}} \right) \cdot Y_n^m(\theta, \phi) \tag{2.5}$$

In the above expansion, the terms $Y_n^m(\theta, \phi) r^n$ are usually referred to as spherical harmonics of degree n, the terms $Y_n^m(\theta, \phi)/r^{n+1}$ are called spherical harmonics of degree $-n - 1$, and the coefficients L_n^m and M_n^m are known as the moments of the expansion.

Remark: It is obvious that in a far field (multipole) expansion, the coefficients L_n^m must be set to zero in order to satisfy the condition that the field decay at infinity. In a local expansion (which is to be analytic in a sphere centered at the origin), it is clearly the coefficients M_n^m which must be set to zero.

Lemmas 2.3 - 2.5 below are well-known. Their proofs can be found, for example, in [9] or [16].

Lemma 2.3.

$$\frac{Y_n^0(\theta, \phi)}{r^{n+1}} = A_n^0 \cdot \frac{\partial^n}{\partial z^n} \left(\frac{1}{r} \right) .$$

For $m > 0$, we have

$$\frac{Y_n^m(\theta,\phi)}{r^{n+1}} = A_n^m \cdot (\frac{\partial}{\partial x} + i\frac{\partial}{\partial y})^m \left(\frac{\partial}{\partial z}\right)^{n-m} \left(\frac{1}{r}\right) ,$$

and

$$\frac{Y_n^{-m}(\theta,\phi)}{r^{n+1}} = A_n^m \cdot (\frac{\partial}{\partial x} - i\frac{\partial}{\partial y})^m \left(\frac{\partial}{\partial z}\right)^{n-m} \left(\frac{1}{r}\right) ,$$

where

$$A_n^m = \frac{(-1)^n}{\sqrt{(n-m)! \cdot (n+m)!}} . \tag{2.6}$$

Remark: The standard definition of the functions $Y_n^m(\theta,\phi)$ includes a normalization factor of

$$\sqrt{2n + 1/4\pi}. \tag{2.7}$$

We will consistently use the definition given above. That is, the coefficient (2.7) will always be omitted.

Since certain differential operators arise frequently in discussions of spherical harmonics, we introduce the following notation.

Definition 2.1. The operators ∂_+, ∂_-, and ∂_z are defined by the expressions

$$\partial_\pm = \frac{\partial}{\partial x} \pm i \cdot \frac{\partial}{\partial y} \quad \text{and}$$

$$\partial_z = \frac{\partial}{\partial z} .$$

Lemma 2.4 *If ϕ is a harmonic function, then*

$$\partial_+\partial_-(\phi) = -\partial_z^2(\phi)$$

Lemma 2.5. *For any $n \geq m \geq 0$,*

$$\partial_\pm^m \partial_z^{n-m} \left(\frac{1}{r}\right) = (-1)^n (n-|m|)! \frac{1}{r^{n+1}} \cdot P_n^{|m|}(\cos\theta) \cdot e^{\pm im\phi} ,$$

where the term $P_n^m(\cos\theta)$ denotes the associated Legendre function of degree n and order m.

Combining lemmas 2.5 and 2.3, we have a useful expression for the spherical harmonics:

$$Y_n^m(\theta,\phi) = \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} \cdot P_n^{|m|}(\cos\theta) e^{im\phi}. \tag{2.8}$$

2.2. The Field Due to Arbitrary Distributions of Charge

We will need a well-known result from the theory of spherical harmonics, which is usually referred to as the Addition Theorem.

Theorem 2.1. *(Addition Theorem for Legendre Polynomials) Let P and Q be points with spherical coordinates (r,θ,ϕ) and (ρ,α,β), respectively, and let γ be the angle subtended between them (Figure 1). Then*

$$P_n(\cos\gamma) = \sum_{m=-n}^{n} Y_n^{-m}(\alpha,\beta)\cdot Y_n^m(\theta,\phi)\ .$$

It is a straightforward matter now to form a multipole expansion describing the far field due to a collection of particles.

Theorem 2.2. **(Multipole Expansion).** *Suppose that m charges of strengths $\{q_i,\ i=1,...,m\}$ are located at the points $\{Q_i=(\rho_i,\alpha_i,\beta_i),\ i=1,...,m\}$, with $|\rho_i|<a$. Then for any $P=(r,\theta,\phi)\in\mathbb{R}^3$ with $r>a$, the potential $\phi(P)$ is given by*

$$\phi(P) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}}\cdot Y_n^m(\theta,\phi)\ , \tag{2.9}$$

where

$$M_n^m = \sum_{i=1}^{m} q_i\cdot\rho_i^n\cdot Y_n^{-m}(\alpha_i,\beta_i). \tag{2.10}$$

Furthermore, for any $p\geq 1$,

$$\left|\phi(P) - \sum_{n=0}^{p}\sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}}\cdot Y_n^m(\theta,\phi)\right| \leq \frac{A}{r-a}\left(\frac{a}{r}\right)^{p+1}\ , \tag{2.11}$$

where

$$A = \sum_{i=1}^{m}|q_i|\ . \tag{2.12}$$

Proof. Let us first consider the contribution from a single charge q_i located at $(\rho_i,\alpha_i,\beta_i)$. From formula (2.1) and the Addition Theorem for Legendre Polynomials, we have

$$\begin{aligned}\phi_i &= \sum_{n=0}^{\infty}\frac{q_i\cdot\rho_i^n}{r^{n+1}}\cdot P_n(\cos\gamma)\\ &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{[q_i\cdot\rho_i^n\cdot Y_n^{-m}(\alpha_i,\beta_i)]}{r^{n+1}}\cdot Y_n^m(\theta,\phi)\ .\end{aligned}$$

The coefficients M_n^m in equation (2.10) are then obtained by superposition. The error bound is an immediate consequence of (2.3), the triangle inequality, and the fact that the ratios ρ_i/r are bounded from above by a/r.

∎

Before proceeding with the further development of the theory of spherical harmonics, we will demonstrate with a simple example how multipole expansions can be used to reduce the computational complexity of the evaluation of potential fields. Suppose that a collection of m point charges of strengths $\{q_i,\ i=1,...,m\}$ are located at the points $\{Q_i=(\rho_i,\alpha_i,\beta_i),\ i=1,\cdots,m\}$, and that $\{P_j=(r_j,\theta_j,\phi_j),\ j=1,\cdots,n\}$ is another set of points in $\mathbb{R}^3$ (Figure 2). We say that the

sets $\{Q_i\}$ and $\{P_j\}$ are *well-separated* if there exist points $P_0, Q_0 \in \mathbf{R}^3$ and a real number $a > 0$ such that

$$\begin{aligned} &\|Q_i - Q_0\| < a \qquad \text{for } i = 1, ..., m\ , \\ &\|P_j - P_0\| < a \qquad \text{for } j = 1, ..., n\ , \quad \text{and} \\ &\|Q_0 - P_0\| > 3a. \end{aligned}$$

In order to obtain the potential at each of the points P_j due to the charges at the points Q_i directly, we could compute

$$\sum_{i=1}^{m} \phi_{Q_i}(P_j) \qquad \text{for } j = 1, ..., n. \tag{2.13}$$

This requires order $n \cdot m$ work (evaluating m fields at n points). Suppose, on the other hand, that we first compute the coefficients of a p^{th}-degree multipole expansion of the potential due to the charges $q_1, q_2, ..., q_m$ about Q_0, using Theorem 2.2. This requires a number of operations proportional to $m \cdot p^2$. Evaluating the resulting multipole expansion at all points P_j requires order $n \cdot p^2$ work, and the total amount of computation is of the order $O(m \cdot p^2 + n \cdot p^2)$. Moreover, by (2.11),

$$\left| \sum_{i=1}^{m} \phi_{Q_i}(P_j) - \sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{M_n^m}{\|P_j - Q_0\|^{n+1}} \cdot Y_n^m(\theta_j, \phi_j) \right| \leq \left(\frac{\sum_{i=1}^{m} |q_i|}{a} \right) \left(\frac{1}{2} \right)^{p+1} ,$$

and in order to obtain a relative precision ϵ (with respect to the total charge), p must be of the order $-\log_2(\epsilon)$. Once the precision is specified, the amount of computation has been reduced to

$$O(m) + O(n)\ ,$$

which is a significant reduction in complexity when compared with the direct method.

2.3. Translation Operators and Error Bounds

As in the two-dimensional case, the principal analytical tools required by the fast algorithm are certain translation operators, acting on both multipole and local expansions. In order to develop the necessary formulae for these procedures, we will need the following three theorems, which can be viewed as generalizations of the classical addition theorem for Legendre polynomials. While a somewhat different form of Theorem 2.5 below can be found in the literature ([6],[3],[15]), Theorems 2.3 and 2.4 appear to be new. The following theorem describes a formula for the expansion of a spherical harmonic of negative degree about a shifted origin.

Theorem 2.3. *(**First Addition Theorem**) Let $Q = (\rho, \alpha, \beta)$ be the center of expansion of an arbitrary spherical harmonic of negative degree. Let the point $P = (r, \theta, \phi)$, with $r > \rho$, and $P - Q = (r', \theta', \phi')$. Then*

$$\frac{Y_{n'}^{m'}(\theta', \phi')}{r'^{n'+1}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{J_m^{m'} \cdot A_n^m \cdot A_{n'}^{m'} \cdot \rho^n \cdot Y_n^{-m}(\alpha, \beta)}{A_{n+n'}^{m+m'}} \cdot \frac{Y_{n+n'}^{m+m'}(\theta, \phi)}{r^{n+n'+1}}\ ,$$

where

$$J_m^{m'} = \begin{cases} (-1)^{min(|m'|,|m|)}, & \text{if } m \cdot m' < 0; \\ 1, & \text{otherwise.} \end{cases} \tag{2.14}$$

Proof. Making use of equation (2.1), the Addition Theorem for Legendre polynomials, and Lemma 2.3, we observe that

$$\begin{aligned}\frac{1}{\|P-Q\|} = \frac{1}{r'} &= \sum_{n=0}^{\infty} \frac{\rho^n}{r^{n+1}} \cdot P_n(\cos\gamma) \\ &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} [\rho^n \cdot Y_n^{-m}(\alpha,\beta)] \cdot \frac{Y_n^m(\theta,\phi)}{r^{n+1}} \\ &= \sum_{n=0}^{\infty} \Big(\sum_{m=-n}^{0} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_n^m \cdot \partial_-^{|m|} \partial_z^{n-|m|} \left(\frac{1}{r}\right) + \\ &\qquad \sum_{m=1}^{n} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_n^m \cdot \partial_+^m \partial_z^{n-m} \left(\frac{1}{r}\right) \Big) .\end{aligned} \tag{2.15}$$

We now consider three separate cases.

Case I : $m' = 0$. From Lemma 2.3,

$$\frac{Y_{n'}^0(\theta',\phi')}{r'^{n'+1}} = A_{n'}^0 \cdot \partial_z^{n'} \left(\frac{1}{r'}\right) . \tag{2.16}$$

Combining (2.15) and (2.16), we obtain

$$\begin{aligned}\frac{Y_{n'}^0(\theta',\phi')}{r'^{n'+1}} &= \sum_{n=0}^{\infty} \Big(\sum_{m=-n}^{0} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^0 \cdot A_n^m \cdot \partial_-^{|m|} \partial_z^{n+n'-|m|} \left(\frac{1}{r}\right) + \\ &\qquad \sum_{m=1}^{n} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^0 \cdot A_n^m \cdot \partial_+^m \partial_z^{n+n'-m} \left(\frac{1}{r}\right) \Big) \\ &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{\rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^0 \cdot A_n^m}{A_{n+n'}^m} \right) \cdot \frac{Y_{n+n'}^m(\theta,\phi)}{r^{n+n'+1}} ,\end{aligned}$$

where the last equality is obtained by another application of Lemma 2.3.

Case II : $m' < 0$. Using Lemma 2.3 again,

$$\begin{aligned}\frac{Y_{n'}^{m'}(\theta',\phi')}{r'^{n'+1}} &= A_{n'}^{m'} \cdot \partial_-^{|m'|} \partial_z^{n'-|m'|} \left(\frac{1}{r'}\right) \\ &= \sum_{n=0}^{\infty} \Big(\sum_{m=-n}^{0} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^{m'} \cdot A_n^m \cdot \partial_-^{|m'|+|m|} \partial_z^{n+n'-|m|-|m'|} \left(\frac{1}{r}\right) + \\ &\qquad \sum_{m=1}^{n} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^{m'} \cdot A_n^m \cdot \partial_-^{|m'|} \partial_+^m \partial_z^{n+n'-m-|m'|} \left(\frac{1}{r}\right) \Big) \\ &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{J_m^{m'} \cdot A_{n'}^{m'} \cdot A_n^m \cdot \rho^n \cdot Y_n^{-m}(\alpha,\beta)}{A_{n+n'}^{m+m'}} \right) \cdot \frac{Y_{n+n'}^{m+m'}(\theta,\phi)}{r^{n+n'+1}} ,\end{aligned}$$

where

$$J_m^{m'} = \begin{cases} 1, & \text{if } m \le 0; \\ (-1)^{min(|m'|,m)}, & \text{if } m > 0. \end{cases}$$

To obtain the last equality, for the terms with $m > 0$, we have used Lemma 2.4 to annihilate whichever of the operators ∂_- and ∂_+ occurs less frequently.

Case III : $m' > 0$. From Lemma 2.3,

$$\begin{aligned}
\frac{Y_{n'}^{m'}(\theta',\phi')}{r'^{n'+1}} &= A_{n'}^{m'} \cdot \partial_+^{m'} \partial_z^{n'-m'} \left(\frac{1}{r'}\right) \\
&= \sum_{n=0}^{\infty} \Bigg(\sum_{m=-n}^{0} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^{m'} \cdot A_n^m \cdot \partial_+^{m'} \partial_-^{|m|} \partial_z^{n+n'-|m|-m'} \left(\frac{1}{r}\right) + \\
&\qquad \sum_{m=1}^{n} \rho^n \cdot Y_n^{-m}(\alpha,\beta) \cdot A_{n'}^{m'} \cdot A_n^m \cdot \partial_+^{m+m'} \partial_z^{n+n'-m-m'} \left(\frac{1}{r}\right) \Bigg) \\
&= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{J_m^{m'} \cdot A_{n'}^{m'} \cdot A_n^m \cdot \rho^n \cdot Y_n^{-m}(\alpha,\beta)}{A_{n+n'}^{m+m'}} \right) \cdot \frac{Y_{n+n'}^{m+m'}(\theta,\phi)}{r^{n+n'+1}} ,
\end{aligned}$$

where

$$J_m^{m'} = \begin{cases} 1, & \text{if } m \geq 0; \\ (-1)^{min(m',|m|)}, & \text{if } m < 0. \end{cases}$$

As before, for the terms with $m < 0$, we have used Lemma 2.4 to annihilate whichever of the operators ∂_- and ∂_+ occurs less frequently.

∎

The second addition theorem yields a formula for converting a spherical harmonic of negative degree (a multipole term) with respect to one origin into a local expansion about a shifted origin.

Theorem 2.4. *(**Second Addition Theorem**) Let $Q = (\rho,\alpha,\beta)$ be the center of expansion of an arbitrary spherical harmonic of negative degree. Let the point $P = (r,\theta,\phi)$, with $r < \rho$ and $P - Q = (r',\theta',\phi')$. Then*

$$\frac{Y_{n'}^{m'}(\theta',\phi')}{r'^{n'+1}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{J_m^{m'} \cdot A_n^m \cdot A_{n'}^{m'} \cdot Y_{n+n'}^{m'-m}(\alpha,\beta)}{\rho^{n+n'+1} \cdot A_{n+n'}^{m-m'}} \cdot Y_n^m(\theta,\phi) r^n ,$$

where

$$J_m^{m'} = \begin{cases} (-1)^{n'}(-1)^{min(|m'|,|m|)}, & \text{if } m \cdot m' > 0; \\ (-1)^{n'}, & \text{otherwise.} \end{cases} \tag{2.17}$$

Proof. We first let (x_P, y_P, z_P) and (x_Q, y_Q, z_Q) denote the Cartesian coordinates of the points P and Q, respectively. Then

$$\begin{aligned}
\frac{\partial}{\partial x_P}\left(\frac{1}{r'}\right) &= -\frac{\partial}{\partial x_Q}\left(\frac{1}{r'}\right) \\
\frac{\partial}{\partial y_P}\left(\frac{1}{r'}\right) &= -\frac{\partial}{\partial y_Q}\left(\frac{1}{r'}\right) \\
\frac{\partial}{\partial z_P}\left(\frac{1}{r'}\right) &= -\frac{\partial}{\partial z_Q}\left(\frac{1}{r'}\right) .
\end{aligned} \tag{2.18}$$

We will denote by $\partial_{+_P}, \partial_{-_P}, \partial_{z_P}, \partial_{+_Q}, \partial_{-_Q}, \partial_{z_Q}$, the differential operators given by Definition 2.1, with respect to the indicated variable point.

Combining equation (2.2), the Addition Theorem for Legendre Polynomials, and Lemma 2.3, we now obtain

$$\begin{aligned}\frac{1}{\|P-Q\|} = \frac{1}{r'} &= \sum_{n=0}^{\infty} \frac{r^n}{\rho^{n+1}} \cdot P_n(\cos\gamma) \\ &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{Y_n^{-m}(\alpha,\beta)}{\rho^{n+1}} \cdot Y_n^m(\theta,\phi) \cdot r^n \\ &= \sum_{n=0}^{\infty} \Big(\sum_{m=-n}^{0} A_n^m \cdot \partial_{+Q}^{|m|} \partial_{z_Q}^{n-|m|} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n + \\ &\qquad \sum_{m=1}^{n} A_n^m \cdot \partial_{-Q}^{m} \partial_{z_Q}^{n-m} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n \Big).\end{aligned}$$

Case I : $m' = 0$. Due to Lemma 2.3 and (2.18), we have

$$\begin{aligned}\frac{Y_{n'}^0(\theta',\phi')}{r'^{n'+1}} &= A_{n'}^0 \cdot \partial_{z_P}^{n'} \left(\frac{1}{r'}\right) \\ &= \sum_{n=0}^{\infty} \Big(\sum_{m=-n}^{0} (-1)^{n'} A_{n'}^0 \cdot A_n^m \cdot \partial_{+Q}^{|m|} \partial_{z_Q}^{n+n'-|m|} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n + \\ &\qquad \sum_{m=1}^{n} (-1)^{n'} A_{n'}^0 \cdot A_n^m \cdot \partial_{-Q}^{m} \partial_{z_Q}^{n+n'-m} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n \Big) \\ &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{(-1)^{n'} A_{n'}^0 \cdot A_n^m \cdot Y_{n+n'}^{-m}(\alpha,\beta)}{\rho^{n+n'+1} \cdot A_{n+n'}^m} \right) \cdot Y_n^m(\theta,\phi) r^n \ ,\end{aligned}$$

where the last equality is obtained from Lemma 2.3.

Case II : $m' < 0$. Using Lemmas 2.3 and 2.4, we have

$$\begin{aligned}\frac{Y_{n'}^{m'}(\theta',\phi')}{r'^{n'+1}} &= A_{n'}^{m'} \cdot \partial_{-P}^{|m'|} \partial_{z_P}^{n'-|m'|} \left(\frac{1}{r'}\right) \\ &= \sum_{n=0}^{\infty} \Big(\sum_{m=-n}^{0} (-1)^{n'} A_{n'}^{m'} \cdot A_n^m \cdot \partial_{-Q}^{|m'|} \partial_{+Q}^{|m|} \partial_{z_Q}^{n+n'-|m|-|m'|} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n + \\ &\qquad \sum_{m=1}^{n} (-1)^{n'} A_{n'}^{m'} \cdot A_n^m \cdot \partial_{-Q}^{|m'|} \partial_{-Q}^{m} \partial_{z_Q}^{n+n'-|m'|-m} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n \Big) \\ &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{J_m^{m'} \cdot A_{n'}^{m'} \cdot A_n^m \cdot Y_{n+n'}^{m'-m}(\alpha,\beta)}{\rho^{n+n'+1} \cdot A_{n+n'}^{m-m'}} \right) \cdot Y_n^m(\theta,\phi) \cdot r^n \ ,\end{aligned}$$

where

$$J_m^{m'} = \begin{cases} (-1)^{n'}, & \text{if } m > 0; \\ (-1)^{n'}(-1)^{\min(|m'|,|m|)}, & \text{if } m < 0. \end{cases}$$

Case III : $m' > 0$. From Lemma 2.3,

$$\begin{aligned}
\frac{Y_{n'}^{m'}(\theta',\phi')}{r'^{n'+1}} &= A_{n'}^{m'} \cdot \partial_{+P}^{m'} \partial_{z_P}^{n'-m'} \left(\frac{1}{r'}\right) \\
&= \sum_{n=0}^{\infty} \Bigg(\sum_{m=-n}^{0} (-1)^{n'} A_{n'}^{m'} \cdot A_n^m \cdot \partial_{+Q}^{m'} \partial_{+Q}^{-m} \partial_{z_Q}^{n+n'-(m'-m)} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n + \\
&\qquad \sum_{m=1}^{n} (-1)^{n'} A_{n'}^{m'} \cdot A_n^m \cdot \partial_{+Q}^{m'} \partial_{-Q}^{m} \partial_{z_Q}^{n+n'-m-m'} \left(\frac{1}{\rho}\right) \cdot Y_n^m(\theta,\phi) \cdot r^n \Bigg) \\
&= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{J_m^{m'} \cdot A_{n'}^{m'} \cdot A_n^m \cdot Y_{n+n'}^{m'-m}(\alpha,\beta)}{\rho^{n+n'+1} \cdot A_{n+n'}^{m-m'}} \right) \cdot Y_n^m(\theta,\phi) \cdot r^n \ ,
\end{aligned}$$

where

$$J_m^{m'} = \begin{cases} (-1)^{n'}, & \text{if } m < 0; \\ (-1)^{n'}(-1)^{min(|m'|,|m|)}, & \text{if } m > 0. \end{cases}$$

As before, for the terms with $m > 0$, we have used Lemma 2.4 to annihilate whichever of the operators ∂_- and ∂_+ occurs less frequently.

∎

The last addition theorem describes a formula for expanding a spherical harmonic of nonnegative degree about a shifted origin. Its proof is similar to those of the first two addition theorems. A more involved proof, based on group representation theory, can be found in [15].

Theorem 2.5. *(**Third Addition Theorem**) Let $Q = (\rho,\alpha,\beta)$ be the center of expansion of an arbitrary spherical harmonic of nonnegative degree. Let the point $P = (r,\theta,\phi)$ with $P - Q = (r',\theta',\phi')$. Then*

$$\frac{Y_{n'}^{m'}(\theta',\phi')}{r'^{n'+1}} = \sum_{n=0}^{n'} \sum_{m=-n}^{n} \frac{J_{n,m}^{m'} \cdot A_n^m \cdot A_{n'-n}^{m'-m} \cdot \rho^n \cdot Y_n^m(\alpha,\beta)}{A_{n'}^{m'}} \cdot Y_{n'-n}^{m'-m}(\theta,\phi) r^{n'-n} \ ,$$

where

$$J_{n,m}^{m'} = \begin{cases} (-1)^n(-1)^m, & \text{if } m \cdot m' < 0; \\ (-1)^n(-1)^{m'-m}, & \text{if } m \cdot m' > 0 \text{ and } |m'| < |m|; \\ (-1)^n, & \text{otherwise.} \end{cases} \tag{2.19}$$

We are in a position now to develop the translation operators which will allow us to manipulate multipole expansions and local expansions in the manner required by the fast algorithm.

Theorem 2.6. *(**Translation of a Multipole Expansion**) Suppose that m charges of strengths $q_1, q_2, \cdots, q_m$ are located inside the sphere D of radius a with center at $Q = (\rho,\alpha,\beta)$, and that for points $P = (r,\theta,\phi)$ outside D, the potential due to these charges is given by the multipole expansion*

$$\Phi(P) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{O_n^m}{r'^{n+1}} \cdot Y_n^m(\theta',\phi') \ , \tag{2.20}$$

where $P - Q = (r',\theta',\phi')$. Then for any point $P = (r,\theta,\phi)$ outside the sphere D_1 of radius $(a+\rho)$,

$$\Phi(P) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} \frac{M_j^k}{r^{j+1}} \cdot Y_j^k(\theta,\phi) \ . \tag{2.21}$$

where

$$M_j^k = \sum_{n=0}^{j} \sum_{m=-n}^{n} \frac{O_{j-n}^{k-m} \cdot J_m^{k-m} \cdot A_n^m \cdot A_{j-n}^{k-m} \cdot \rho^n \cdot Y_n^{-m}(\alpha, \beta)}{A_j^k} , \tag{2.22}$$

with J_r^s and A_r^s defined by equations (2.14) and (2.6), respectively. Furthermore, for any $p \geq 1$,

$$\left| \Phi(P) - \sum_{j=0}^{p} \sum_{k=-j}^{j} \frac{M_j^k}{r^{j+1}} \cdot Y_j^k(\theta, \phi) \right| \leq \left(\frac{\sum_{i=1}^{m} |q_i|}{r - (a+\rho)} \right) \left(\frac{a+\rho}{r} \right)^{p+1} . \tag{2.23}$$

Proof. The coefficients of the shifted expansion (2.21) are obtained by applying the First Addition Theorem to each of the terms in the original expansion (2.20). For the error bound (2.23), observe that the terms M_n^m are the coefficients of the (unique) multipole expansion about the origin of those charges contained in the sphere D, and Theorem 2.2 applies with a replaced by $a + \rho$. ∎

The second translation procedure is used to convert a multipole expansion of the field induced by a collection of charges into a local expansion inside some region of analyticity.

Theorem 2.7. *(**Conversion of a Multipole Expansion into a Local Expansion**) Suppose that m charges of strengths $q_1, q_2, \cdots, q_m$ are located inside the sphere D_Q of radius a with center at $Q = (\rho, \alpha, \beta)$, and that $\rho > (c+1)a$ with $c > 1$ (Figure 3). Then the corresponding multipole expansion (2.20) converges inside the sphere D_0 of radius a centered at the origin. Inside D_0, the potential due to the charges $q_1, q_2, \cdots, q_m$ is described by a local expansion:*

$$\Phi(P) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} L_j^k \cdot Y_j^k(\theta, \phi) \cdot r^j , \tag{2.24}$$

where

$$L_j^k = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{O_n^m \cdot J_k^m \cdot A_n^m \cdot A_j^k \cdot Y_{j+n}^{m-k}(\alpha, \beta)}{A_{j+n}^{m-k} \cdot \rho^{j+n+1}} , \tag{2.25}$$

with J_r^s and A_r^s defined by equations (2.17) and (2.6), respectively. Furthermore, for any $p \geq 1$,

$$\left| \Phi(P) - \sum_{j=0}^{p} \sum_{k=-j}^{j} L_j^k \cdot Y_j^k(\theta, \phi) \cdot r^{j+1} \right| \leq \left(\frac{\sum_{i=1}^{m} |q_i|}{ca - a} \right) \left(\frac{1}{c} \right)^{p+1} . \tag{2.26}$$

Proof. We obtain the coefficients of the local expansion (2.24) by applying the Second Addition Theorem to each of the terms in the multipole expansion (2.20). The bound (2.26) is an immediate consequence of the simpler error bound (2.4) and the triangle inequality. ∎

The following theorem yields a procedure for shifting the origin of a truncated local expansion. It is an exact translation, and no error bound is needed.

Theorem 2.8. *(**Translation of a Local Expansion**)*
Let $Q = (\rho, \alpha, \beta)$ be the origin of a local expansion

$$\Phi(P) = \sum_{n=0}^{p} \sum_{m=-n}^{n} O_n^m \cdot Y_n^m(\theta', \phi') \cdot r'^n , \tag{2.27}$$

where $P = (r, \theta, \phi)$ *and* $P - Q = (r', \theta', \phi')$. *Then*

$$\Phi(P) = \sum_{j=0}^{p} \sum_{k=-j}^{j} L_j^k \cdot Y_j^k(\theta, \phi) \cdot r^j \ , \tag{2.28}$$

where

$$L_j^k = \sum_{n=j}^{p} \sum_{m=-n}^{n} \frac{O_n^m \cdot J_{n-j,m-k}^m \cdot A_{n-j}^{m-k} \cdot A_j^k \cdot Y_{n-j}^{m-k}(\alpha, \beta) \cdot \rho^{n-j}}{A_j^k} \ . \tag{2.29}$$

with $J_{r,s}^t$ *and* A_r^s *defined by equations (2.19) and (2.6), respectively.*

Proof. The coefficients (2.29) are obtained by applying the Third Addition Theorem to each of the terms in the expansion (2.27).

∎

3. The Fast Multipole Algorithm

In this section, we present an algorithm for the rapid evaluation of the potentials and/or electrostatic fields due to distributions of charges. The central strategy used is that of clustering particles at various spatial lengths and computing interactions with other clusters which are sufficiently far away by means of multipole expansions. Interactions with particles which are nearby are handled directly.

To be more specific, let us consider the geometry of the computational box, depicted in Figure 4. It is a cube with sides of length one, centered about the origin of the coordinate system, and is assumed to contain all N particles of the system under consideration.

Fixing a precision ϵ, we choose $p \approx log_2(\epsilon)$ and specify that no interactions be computed for clusters of particles which are not well-separated. This is precisely the condition needed for the error bounds (2.11),(2.23) and (2.26) to apply with $c = 2$, the truncation error to be bounded by 2^{-p}, and the desired precision to be achieved. In order to impose such a condition, we introduce a hierarchy of meshes which refine the computational box into smaller and smaller regions (Figure 4). Mesh level 0 is equivalent to the entire box, while mesh level $l + 1$ is obtained from level l by subdivision of each region into eight equal parts. The number of distinct boxes at mesh level l is equal to 8^l. A tree structure is imposed on this mesh hierarchy, so that if *ibox* is a fixed box at level l, the eight boxes at level $l + 1$ obtained by subdivision of *ibox* are considered its children.

Other notation used in the description of the algorithm includes

nearest neighbor	For box i at level l, a nearest neighbor is a box at the same level of refinement which shares a boundary point with box i.
second nearest neighbor	For box i at level l, a second nearest neighbor is a box at the same level of refinement which shares a boundary point with a nearest neighbor of box i.
$\Phi_{l,i}$	the p^{th}-order multipole expansion (about the box center) of the potential field created by the particles contained inside box i at level l,
$\Psi_{l,i}$	the p^{th}-order local expansion about the center of box i at level l, describing the potential field due to all particles outside the box and its nearest and second nearest neighbors.

$\tilde{\Psi}_{l,i}$ — the p^{th}-order local expansion about the center of box i at level l, describing the potential field due to all particles outside i's *parent* box and the *parent* box's nearest and second nearest neighbors.

Interaction list: for box i at level l, it is the set of boxes which are children of the nearest and second nearest neighbors of i's parent and which are not nearest or second nearest neighbors of box i.

Suppose now that at level $l-1$, the local expansion $\Psi_{l-1,i}$ has been obtained for all boxes. Then, by using Theorem 2.6 to shift (for all i) the expansion $\Psi_{l-1,i}$ to each of box i's children, we have, for each box j at level l, a local representation of the potential due to all particles outside of j's parent's neighbors, namely $\tilde{\Psi}_{l,j}$. The interaction list is, therefore, precisely that set of boxes whose contribution to the potential must be added to $\tilde{\Psi}_{l,j}$ in order to create $\Psi_{l,j}$. This is done by using Theorem 2.7 to convert the multipole expansions of these interaction boxes to local expansions about the current box center and adding them to the expansion obtained from the parent. Note also that with free-space boundary conditions, $\Psi_{0,i}$ and $\Psi_{1,i}$ are equal to zero since there are no well-separated boxes to consider, and we can begin forming local expansions at level 2.

Following is a formal description of the algorithm.

Algorithm

Initialization

Choose a level of refinement $n \approx \log_8 N$, a precision ϵ, and set $p \approx \log_2(\epsilon)$.

Upward Pass

Step 1

Comment [Form multipole expansions of potential field due to particles in each box about the box center at the finest mesh level.]

do $ibox = 1, ..., 8^n$
  Form a p^{th}-degree multipole expansion $\Phi_{n,ibox}$, by using Theorem 2.2.
enddo

Step 2

Comment [Form multipole expansions about the centers of all boxes at all coarser mesh levels, each expansion representing the potential field due to all particles contained in one box.]

do $l = n-1, ..., 0$
  do $ibox = 1, ..., 8^l$
    Form a p^{th}-degree multipole expansion $\Phi_{l,ibox}$, by using Theorem 2.6 to shift the center of each child box's expansion to the current box center and adding them together.
  enddo
enddo

Downward Pass

Comment [In the downward pass, interactions are consistently computed at the coarsest possible level. For a given box, this is accomplished by including interactions with those boxes which are well-separated and whose interactions have not been accounted for at the parent's level.]

Step 3

Comment [Form a local expansion about the center of each box at each mesh level $l \leq n-1$. This local expansion describes the field due to all particles in the system that are not contained in the current box or its nearest neighbors. Once the local expansion is obtained for a given box, it is shifted, in the second inner loop to the centers of the box's children, forming the initial expansion for the boxes at the next level.]

Set $\tilde{\Psi}_{1,1} = \tilde{\Psi}_{1,2} = \cdots = \tilde{\Psi}_{1,8} = (0, 0, ..., 0)$
do $l = 1, ..., n-1$
  do $ibox = 1, ..., 8^l$
    Form $\Psi_{l,ibox}$ by using Theorem 2.7 to convert the multipole expansion $\Phi_{l,j}$ of each box j in *interaction list* of box $ibox$ to a local expansion about the center of box $ibox$, adding these local expansions together, and adding the result to $\tilde{\Psi}_{l,ibox}$.
  enddo

  do $ibox = 1, ..., 8^l$
    Form the expansion $\tilde{\Psi}_{l+1,j}$ for $ibox$'s children by using Theorem 2.8 to expand $\Psi_{l,ibox}$ about the children's box centers.
  enddo
enddo

Step 4

Comment [Compute interactions at finest mesh level]

do $ibox = 1, ..., 8^n$
    Form $\Psi_{l,ibox}$ by using Theorem 2.7 to convert the multipole expansion $\Phi_{l,j}$ of each box j in *interaction list* of box $ibox$ to a local expansion about the center of box $ibox$, adding these local expansions together, and adding the result to $\tilde{\Psi}_{l,ibox}$.
enddo

Comment [Local expansions at finest mesh level are now available. They can be used to generate the potential or force due to all particles outside the nearest neighbor boxes at finest mesh level.]

Step 5

Comment [Evaluate local expansions at particle positions.]

do $ibox = 1, ..., 8^n$
  For every particle p_j located at the point P_j in box $ibox$, evaluate $\Phi_{n,ibox}(P_j)$.
enddo

Step 6

Comment [Compute potential (or force) due to nearest neighbors directly.]

do $ibox = 1, ..., 8^n$
For every particle p_j in box $ibox$, compute interactions with all other particles within the box and its nearest and second nearest neighbors.
enddo

Step 7

do $ibox = 1, ..., 8^n$
For every particle in box $ibox$, add direct and far-field terms together.
enddo

Remark: Each local expansion is described by its p^2 coefficients. Direct evaluation of this expansion at a point yields the potential. But the force can be obtained from the gradient of the local expansion, and these partial derivatives are available analytically. There is no need for numerical differentiation. Furthermore, since the components of $\nabla\Phi$ are themselves harmonic, there exist error bounds for the force of exactly the same form as (2.11),(2.23) and (2.26).

A brief analysis of the algorithmic complexity is given below.

Step Number	*Operation Count*	*Explanation*
Step 1	order Np^2	each particle contributes to one expansion at the finest level.
Step 2	order Np^4	At the l^{th} level, 8^l shifts involving order p^4 work per shift must be performed.
Step 3	order $\leq 876Np^4$	There are at most 875 entries in the interaction list for each box at each level. An extra order Np^4 work is required for the second loop.
Step 4	order $\leq 875Np^4$	Again, there are at most 875 entries in the interaction list for each box and $\approx N$ boxes.
Step 5	order Np^2	One p^{th}-degree expansion is evaluated for each particle.
Step 6	order $\frac{25}{2}Nk_n$	Let k_n be a bound on the

		number of particles per box at the finest mesh level. Interactions must be computed within the box and its eight nearest neighbors, but using Newton's third law, we need only compute half of the pairwise interactions.
Step 7	order N	Adding two terms for each particle.

The estimate for the running time is therefore

$$N \cdot (a \cdot (log_2(\epsilon))^2 + b \cdot (log_2(\epsilon))^4 + d \cdot k_n + e) \ ,$$

with the constants a, b, c, d, and e determined by the computer system, language, implementation, etc.

Remark:

In addition to the asymptotic time complexity, asymptotic storage requirements are an important characteristic of a numerical procedure. The algorithm requires that $\Phi_{l,j}$ and $\Psi_{l,j}$ be stored, as well as the locations of the particles, their charges, and the results of the calculations (the potentials and/or electric fields). Since every box at every level has a pair of p^{th}-degree expansions, Φ and Ψ, associated with it, and the lengths of all other storage arrays are proportional to N, it is easy to see that the asymptotic storage requirements of the algorithm are of the form

$$(\alpha + \beta \cdot p^2) \cdot N \ , \quad \text{or}$$

$$(\alpha + \beta \cdot (log_2(\epsilon))^2 \cdot N \ ,$$

with the coefficients α and β determined, as above, by the computer system, language, implementation, etc.

Remark: It is clear that the operation count for Step 6 that the algorithm assumes a reasonably homogeneous distribution of particles. If the distribution were highly non-homogeneous, then we would need to refine only those portions of space where the number of particles is large. Although its description is more involved, an adaptive version retains both the accuracy and the computational speed of the algorithm (see [4]).

4. Conclusions

An order $O(N)$ algorithm has been constructed for the evaluation of Coulombic fields and potentials in large-scale ensembles of particles in three dimensions. The algorithm generalizes our earlier two-dimensional results (see [7],[8]) and retains both the general structure and the asymptotic complexity of its predecessor. Here, we present a description of the procedure and its complexity analysis. Numerical experiments are currently being conducted with a computer implementation of the algorithm, and the results of these experiments will be reported in the near future.

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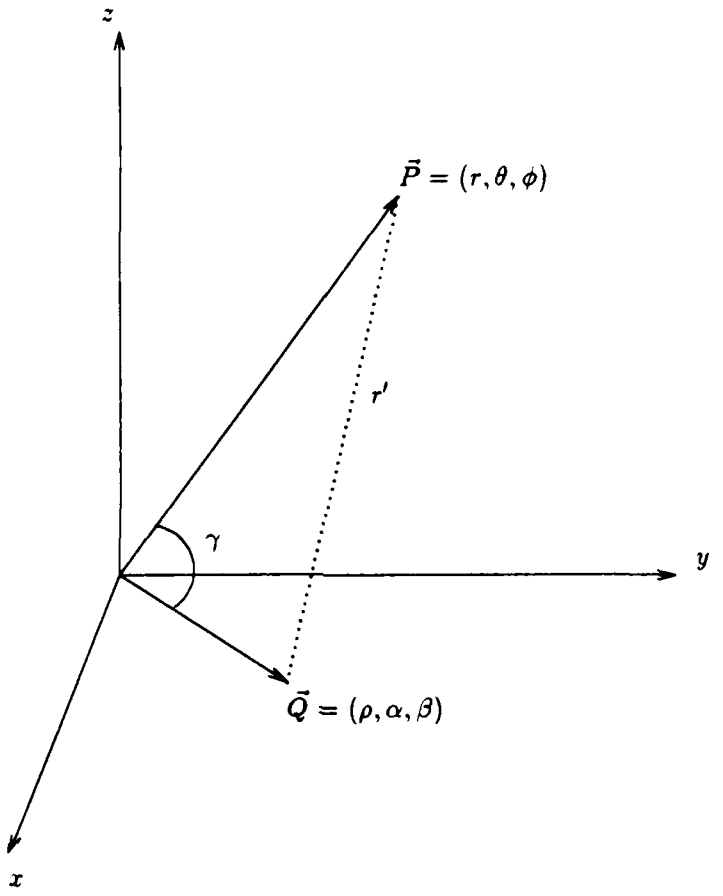

Figure 1: Points $\vec{P}$ and $\vec{Q}$ separated by a distance r', and subtending an angle γ between them.

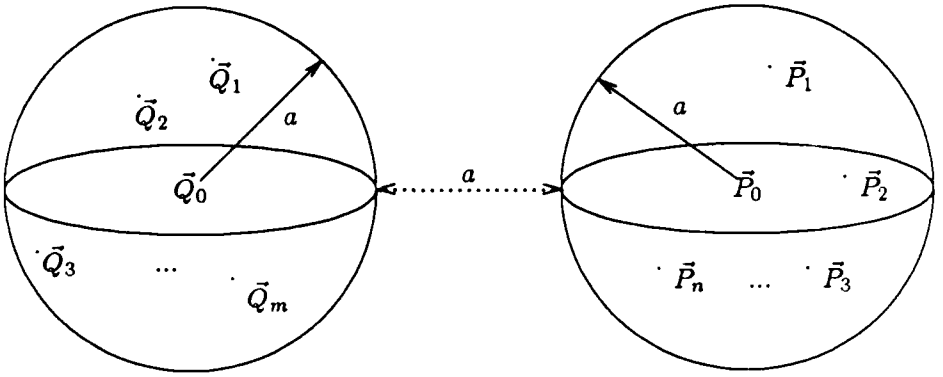

Figure 2: Well-separated sets in $\mathbf{R}^3$.

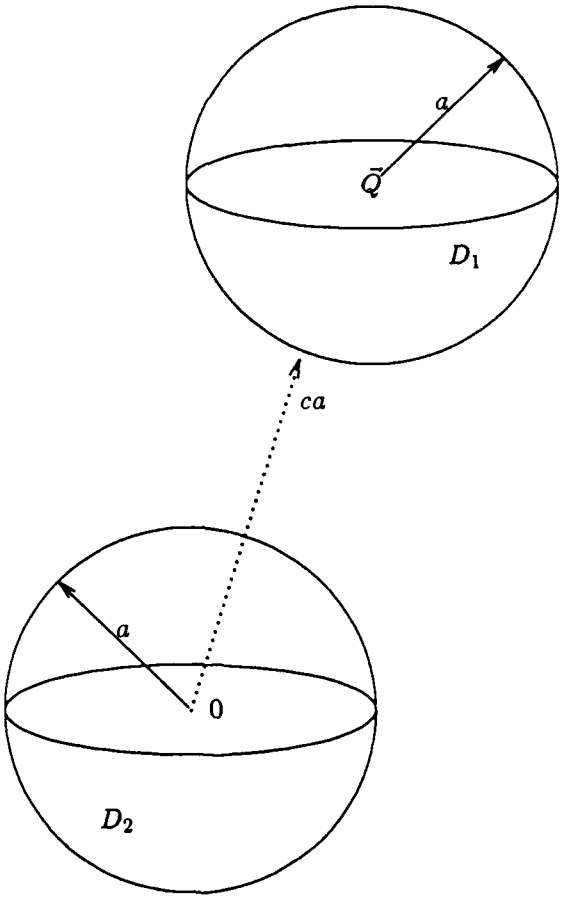

Figure 3: Source charges $q_1, q_2, ..., q_l$ are contained in the sphere D_1. The corresponding multipole expansion about $\vec{Q}$ converges inside D_2.

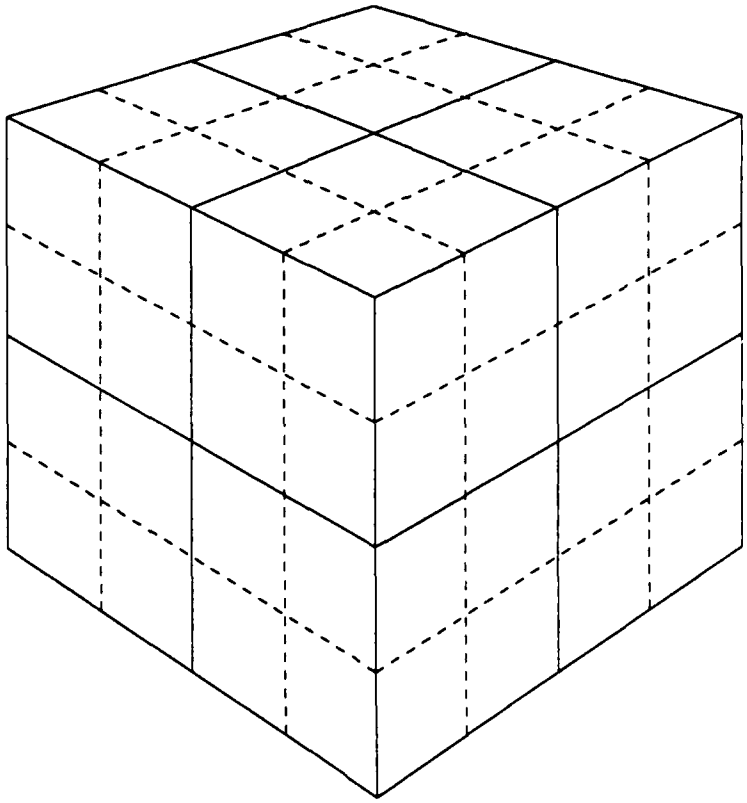

Figure 4: The computational box and the first two levels of refinement, inducated by the solid and dashed lines, respectively.

END

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